Formyl chloride

2565-30-2 | DTXSID30180344

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 22.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.78e-01

Confidence level: 7.15e-01

Nearest Neighbors from the Training Set

Image not found
Dichloromethane
Measured: 27.5
Predicted: 34.9

Image not found
Methyl bromide
Measured: 21.9
Predicted: 27.5

Image not found
1,1-Dichloroethylene
Measured: 64.6
Predicted: 58.2

Image not found
Methyl isothiocyanate
Measured: 9.33
Predicted: 7.63

Image not found
2,2,2-Trichloroacetamide
Measured: 9.77
Predicted: 6.26